1. **Record Nr.**   UNISA996390325903316

   Titolo   Orders conceived and published by the Lord Major and aldermen of the city of London, concerning the infection of the plague [[electronic resource]]

   Pubbl/distr/stampa [London], : Printed by James Flesher .., [1665]

   Descrizione fisica [15] p

   Soggetti   Plague - England - London
                           London (England) History 17th century

   Lingua di pubblicazione Inglese

   Formato   Materiale a stampa

   Livello bibliografico Monografia

   Note generali   Reproduction of original in Huntington Library.
                           Identified as STC 16729 in reel guide.

   Sommario/riassunto eebo-0113

2.	Record Nr.	UNINA9910891283803321
	Titolo	Annales Universitatis Mariae Curie-Skodowska . Sectio AI Informatica
	Pubbl/distr/stampa	Lublin, Polonia : , : Uniwersytet Marii Curie-Skodowskiej
	ISSN	2083-3628
	Descrizione fisica	1 online resource
	Soggetti	Computer science Periodicals.
	Lingua di pubblicazione	Inglese
	Formato	Materiale a stampa
	Livello bibliografico	Periodico
	Note generali	Refereed/Peer-reviewed Also published: Warsaw, Poland : Versita, 2011-2013; Warsaw, Poland : De Gruyter Open, 2014-
3.	Record Nr.	UNINA9911019830803321
	Titolo	Computational spectroscopy : methods, experiments and applications / / edited by Jorg Grunenberg
	Pubbl/distr/stampa	Weinheim, : Wiley-VCH Chichester, : John Wiley [distributor], c2010
	ISBN	9786612849565 9783527643622 3527643621 9781282849563 1282849565 9783527633272 3527633278 9783527633289 3527633286
	Edizione	[4th ed.]
	Descrizione fisica	1 online resource (434 p.)
	Altri autori (Persone)	GrunenbergJorg
	Disciplina	543.5
	Soggetti	Molecular spectroscopy - Data processing Spectrum analysis - Data processing

Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Computational Spectroscopy: Methods, Experiments and Applications; Contents; Preface; List of Contributors; 1 Concepts in Computational Spectrometry: the Quantum and Chemistry; 1.1 Introduction; 1.2 Quantum Laws, or the Laws of Discreteness; 1.3 Quantum Theories of a Harmonic Oscillator; 1.3.1 Matrix Mechanics; 1.3.2 Wave Mechanics; 1.3.3 Dirac.s Operators for Creation and Destruction; 1.3.4 Discussion of Quantum Theories in Relation to an Harmonic Oscillator; 1.4 Diatomic Molecule as Anharmonic Oscillator; 1.5 Quantum Mechanics and Molecular Structure; 1.6 Conclusions; References 2 Computational NMR Spectroscopy2.1 Introduction; 2.2 NMR Properties; 2.3 Chemical Shifts; 2.4 NICS and Aromaticity; 2.5 Spin-Spin Coupling Constants; 2.6 Solvent Effects; 2.7 Conclusions; 2.8 The Problem of the Error in Theoretical Calculations of Chemical Shifts and Coupling Constants; References; 3 Calculation of Magnetic Tensors and EPR Spectra for Free Radicals in Different Environments; 3.1 Introduction; 3.2 The General Model; 3.3 Spin Hamiltonian, g-Tensor, Hyperfine Coupling Constants, and Zero-Field Splitting; 3.3.1 The Spin Hamiltonian; 3.3.2 Electronic Structure Theory 3.3.3 Additional Terms in the Hamiltonian3.3.4 Linear Response Theory; 3.3.5 Linear Response Equations for Spin Hamiltonian Parameters; 3.3.6 Computational Aspects: Functionals and Basis Sets; 3.4 Stereoelectronic, Environmental, and Dynamical Effects; 3.4.1 Structures and Magnetic Parameters; 3.4.2 Environmental Effects; 3.4.3 Short-Time Dynamical Effects; 3.5 Line Shapes; 3.6 Concluding Remarks; References; 4 Generalization of the Badger Rule Based on the Use of Adiabatic Vibrational Modes; 4.1 Introduction; 4.2 Applicability of Badger-Type Relationships in the Case of Diatomic Molecules 4.3 Dissection of a Polyatomic Molecule into a Collection of Quasi-Diatomic Molecules: Local Vibrational Modes4.3.1 Localized Vibrational Modes; 4.3.2 The Adiabatic Internal Coordinate Modes; 4.3.3 Properties of Adiabatic Internal Coordinate Modes; 4.3.4 Characterization of Normal Modes in Terms of AICoMs; 4.3.5 Advantages of AICoMs; 4.4 Local Mode Properties Obtained from Experiment; 4.4.1 Isolated Stretching Modes; 4.4.2 Local Mode Frequencies from Overtone Spectroscopy; 4.4.3 Local Mode Information via an Averaging of Frequencies: Intrinsic Frequencies; 4.4.4 Compliance Force Constants 4.5 Badger-type Relationships for Polyatomic Molecules4.6 Conclusions; References; 5 The Simulation of UV-Vis Spectroscopy with Computational Methods; 5.1 Introduction; 5.2 Quantum Mechanical Methods; 5.3 Modeling Solvent Effects; 5.4 Toward the Simulation of UV-Vis Spectra; 5.5 Some Numerical Examples; 5.6 Conclusions and Perspectives; References; 6 Nonadiabatic Calculation of Dipole Moments; 6.1 Introduction; 6.2 The Molecular Hamiltonian; 6.3 Symmetry; 6.4 The Hellmann-Feynman Theorem; 6.5 The Born-Oppenheimer Approximation; 6.6 Interaction between a Molecule and an External Field 6.7 Experimental Measurements of Dipole Moments
Sommario/riassunto	Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years, from single molecule studies to the simulation of clusters

and the solid state, from organic molecules to complex inorganic systems and from basic research to commercial applications in the area of environment relevance. In so doing, it covers a multitude of apparatus-driven technologies, starting with the common and traditional spectroscopic methods, more recent developments (THz)